Hydrodynamic electron-transport model: Nonparabolic corrections to the streaming terms

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This paper presents a hydrodynamic model suitable for studying hot-electron transport in semiconducting materials with nonparabolic conduction bands. The model presented is based upon a unique derivation of the moments of the Boltzmann-transport equation for the streaming (collision-independent) terms. This derivation implements an efficient and compact mathematical formalism appropriate for electrons under the influence of high electric fields and nonstationary conditions. The theoretical investigation also introduces a distributional form with nonparabolic properties to precisely define the resulting nonparabolic *streaming* parameters. The final set of model equations is exhibited in a fashion to clearly show the correction factors to the more familiar hydrodynamic model applicable for the constant-effective-mass case. In general, the hydrodynamic (or conservation) model contains *pure transport* terms that are treated as being independent of the specific dissipation mechanisms and *collision* terms to directly account for the influence of scattering. Since the collision terms are *almost* always treated phenomenologically using a relaxation-time approximation, our formulation of the streaming terms should significantly improve the overall accuracy of the approach. In addition, this paper presents the results of an extensive investigation of the assumed ansatz distribution and resulting nonparabolic-model parameters using an elaborate Monte Carlo model. The Monte Carlo technique was used to generate comparison electron distributions and exact values for the nonparabolic transport parameters for stationary and nonstationary electronic structures. In all cases, excellent agreement was found between the Monte Carlo–calculated parameters and the derived nonparabolic-model terms. The Monte Carlo calculations also revealed that the ansatz distribution used in the derivation represented a significant improvement over the more familar displaced Maxwellian. Therefore, this model should prove very valuable for studying electronic-device structures operating under high-bias conditions.

I. INTRODUCTION

During the past two decades there has been an increased use of hydrodynamic conservation models to investigate nonstationary and nonequilibrium electron dynamics in submicrometer semiconductor devices.[1–14] These models, referred to by some[15,16] as the hydrodynamic equations due to their similarity to the Euler equations of fluid dynamics[17,18] used in classical hydrodynamics studies, are based upon higher moments of the Boltzmann-transport equation (BTE). The popularity of the hydrodynamic electron transport theory is due to the physical and practical attributes of the approach. The hydrodynamic models have the capability to include nonstationary and hot-electron effects[19] and hence are superior to simple drift-diffusion (extreme thermal equilibrium approximation[20] and local-electric-field-dependent case) models. While Monte Carlo methods that solve the full BTE can easily incorporate complicated band structures and detailed scattering rates, hydrodynamic models require much less computation time to generate solutions and possess macroscopic terms which offer important physical insight. Thus the hydrodynamic approach offers much flexibility for future theoretical electron device studies.

Stratton[20] introduced the general conservation or momentum-energy balance approach to investigate hot-electron transport in semiconductors. The analysis performed by Stratton utilized a spherical harmonic expansion with the relaxation-time approximation to define a nonequilibrium distribution which was only slightly anisotropic. This analysis replaced the nonequilibrium distribution by a Maxwellian distribution function in some terms of the BTE. Thus some of the streaming terms in the final transport equations were suppressed. Blotekjaer[21] extended the theory, using a more general analysis which retained all terms of the moment equations, and derived relations applicable to a two-valley semiconductor. These previous investigations were applicable to semiclassical transport and assumed homogeneous materials with parabolic conduction bands.

Since the early work of Stratton and of Blotekjaer, the hydrodynamic approach has been utilized extensively to study various transport phenomena in many different Si,[6,9,22] GaAs,[1,23,24] and heterostructure[11,25,26] electron devices. The particular material, device configuration, and bias conditions under consideration have led to a variety of acceptable simplifications and to a hierarchy of approximate electron-transport models (for example, see Sandborn, Rao, and Blakely[27] and references therein). Also, much effort has been directed toward developing numerical techniques to solve the hydrodynamic transport model self-consistently with Poisson's equation for many semiconductor structures. This has included methods for solving the problem with and without time dependency and in multiple space dimensions[28–30] as well

as an interest in special mathematical problems such as shock waves[31] and acceptable boundary conditions.[32]

Recently, investigations into complex electronic structures have led to a dramatic evolution of the hydrodynamic electron-transport theory. Widiger *et al.*[26] developed a hydrodynamiclike model suitable for studying high-electron-mobility transistors which included both hot-electron effects and conduction outside the quantum subband system. This model was based on an approximate form of the first four moments of the BTE similar to that of Stratton. Azoff[15] incorporated the heterojunction energy-band rules of Marshak and Van Vliet[33] to the hydrodynamic transport equations and used this model to study $Al_xGa_{1-x}As/GaAs$ heterojunction bipolar transistors. This model was based on the first three moments of the BTE with a Fourier law relation used to terminate the moments and generate an approximate form more valid for the general nonequilibrium transport case.

Grubin and Kreskovsky[16] constructed a set of quantum balance *hydrodynamic* equations applicable for electron transport in mescoscopic structures. Their model was derived from the general moment equations of Stroscio[34] using the displaced nonequilibrium Wigner distribution function of Ancona and Iafrate.[35] In their paper, the first two quantum balance equations were applied to a resonant tunneling diode and solutions were generated which showed the occurrence of a negative differential region. Later, Woolard *et al.*[36] presented solutions for the full quantum balance equations applied to an ultrasmall electron device analogous to that of Grubin and Kreskovsky. These results showed that the quantum potential, which was incorporated through density gradients, partially canceled the effects of the barrier potentials to permit carrier transport even though a classical solution did not exist.

There has also been interest in improving the accuracy of hydrodynamic models for high-field applications where electron energies may become very large and the electron gas may reside far from equilibrium. Stewart and Churchill[37] have recently introduced a fully nonparabolic hydrodynamic model for describing hot-electron transport in GaAs. This model attempts to account for nonparabolicity and general distribution functions which become important for the extreme nonequilibrium or hot-electron transport case. However, this analysis includes the introduction of heuristic effective-mass parameters which are necessary to relate average momentum to average velocity as well as relating an effective scalar temperature to thermal and displacement kinetic-energy components. Furthermore, it is necessary to derive this effective mass from stationary Monte Carlo calculations. Also, Azoff[25] has developed a model for electron transport in nonparabolic degenerate semiconductor heterostructures. This analysis, which simultaneously addressed the issues of position-dependent energy bands, high-field energy-band effects, and degenerate statistics, is based on the first four moments of the relaxation-time approximation Boltzmann-transport equation. However, the results presented were primarily restricted to the thermal equilibrium limit with many transport terms derived from approximate thermodynamic principles such as electronic heat capacity and the isothermal approximation. Also, the choice of moment operators and subsequent approximations for this nonparabolic analysis lead to a less than optimum form for comparing the results for the nonparabolic case to the general parabolic hydrodynamic transport equations.

Except for the last few examples, most of the current hydrodynamic transport models either directly or indirectly assume electron transport occurs in parabolic conduction bands and that this ensemble of electrons have the form of a displaced Maxwellian $\mathbf{k}$-space distribution.[27] However, neither of these assumptions is valid for most high-mobility compound semiconductors (such as GaAs) under moderately high electric fields.[37–39] Previously, we presented a hydrodynamic model[39] that accounted for both nonparabolicity and nondisplaced Maxwellian distribution functions. This model made the extreme heuristic assumption that the effective mass, temperature tensors, and heat flow vector could be described by stationary Monte Carlo–generated parameters which only possessed energy dependence. Subsequently, simulations using this model[24] indicated that including a dependence on the displacement component[40] of the kinetic energy was important both physically and in regard to generating stable numerical solutions to the problem. Hence the goal of this paper is to develop a more general transport model which is less dependent on externally generated transport parameters and which approximates hot-electron transport well in nonparabolic semiconductor conduction bands.

This paper presents an alternate formalism for deriving a nonparabolic hydrodynamic transport model that can model hot-electron transport in semiconductors. Section II presents an approach for deriving this model. The model equations are developed by applying a unique set of moment operators [$\Phi_0(\mathbf{k})=1$; a constant, $\Phi_1(\mathbf{k})=\mathbf{u}(\mathbf{k})$; the nonparabolic velocity $\Phi_2(\mathbf{k})=\frac{1}{2}m(\mathbf{k})\mathbf{u}(\mathbf{k})\cdot\mathbf{u}(\mathbf{k})\approx E(\mathbf{k})$; an approximation to the particle energy] to the collisionless Boltzmann-transport equation. The operators, used in this analysis, represent a significant improvement in the development of the hydrodynamic transport model since they lead to a more compact mathematical form. This resulting form can be manipulated more easily and reveals clearly the allowable simplifying approximations. Together, the operators and acceptable approximations lead to a model that is primarily in terms of the familiar averages; electron concentration, average electron velocity, and average electron energy. The remaining integral terms involve only average velocity, momentum space velocity, and a momentum space effective-mass term. This compact nature is utilized later to develop an appropriate physical and mathematical closure for the system.

In this analysis, specific collision terms are omitted. This is done to permit a concise focus on the streaming (collision-independent) terms which evolve from the application of nonparabolic conduction bands. In general, macroscopic models (hydrodynamic, drift-diffusion, etc.) used to approximate electron dynamics in semiconductors contain *pure transport* terms which are considered in-

dependent of the specific dissipation mechanisms.[20,21,27] In fact, dissipation does play a role in determining the final form for some of the streaming terms. The effects of scattering on these terms are introduced through certain characteristics of the final electron distribution function (see Sec. III). This fact prohibits an exact macroscopic treatment for arbitrary electron-transport phenomena. Fortunately, electron transport can be adequately modeled, in many device structures, by establishing *approximate* collision-invariant streaming terms.[9,22] This approach allows the question of how nonparabolic bands and specific scattering mechanisms affect the average loss terms to be addressed as a completely separate issue. Therefore this course is taken to simplify the current presentation. The collision terms, which are *almost* always treated phenomenologically using a relaxation-time approximation, have been developed for a nonparabolic multivalley system (GaAs) and presented elsewhere.[41]

The system of equations, which result from Sec. II, requires an additional mathematical closure before it can be used to study electron transport. In Sec. III, an intuition-based distribution function is proposed as a constitutive (essential) relation to close the moment equations. This ansatz nonparabolic distribution function, which is derived in velocity space for mathematical convenience and approximates some of the characteristics of the true nonparabolic distribution function, is then analyzed and used to develop a set of transport parameters. These resultant transport parameters are shown to depend only on the nonparabolicity parameter and physical quantities: electron concentration, average electron velocity, and average electron energy.

Throughout Secs. II and III, efforts are made to retain a mathematical form that is similar to the full hydrodynamic transport equations applicable to parabolic bands and a displaced Maxwellian distribution function. This more basic model, which has been widely utilized to study electronic devices, has become very familiar to the scientific community interested in transport in semiconductors. This similarity of the present model to the more familiar form should assist in illustrating the primary effects of nonparabolicity on the hydrodynamic transport equations and on how nonparabolicity will affect macroscopic electron transport.

The results from two independent Monte Carlo transport models[42,43] are used in Sec. IV to evaluate the nonparabolic transport parameters. Both Monte Carlo models were used to study transport in GaAs and included most of the important scattering mechanisms. These models were used to investigate electron transport in both stationary (uniform electric field) and nonstationary (ballistic diode) environments. The results of these studies show that there is excellent agreement between this nonparabolic transport model and the Monte Carlo calculations. Hence this nonparabolic transport model presents a viable alternative to studying realistic electronic-device structures operating under high-bias conditions.

II. GENERAL MOMENT EQUATIONS

Consider the collisionless Boltzmann transport equation in terms of the phase-space variables $(\mathbf{r},\mathbf{k},t)$. The developments presented here are independent of the specific scattering phenomena which will be addressed later. Hence the BTE is

$$\frac{\partial f}{\partial t}+\mathbf{u}\cdot\nabla_{\mathbf{r}}f+\frac{\mathbf{F}}{\hbar}\cdot\nabla_{\mathbf{k}}f=0\ , \tag{1}$$

where $f(\mathbf{r},\mathbf{k},t)$ is some arbitrary electron distribution function. Invoking the effective-mass theorem[44] (also called the quasi-free particle approximation[45]) for electron motion defines the electron moment as $\mathbf{p}=\hbar\mathbf{k}$ and identifies the electron group velocity as

$$\frac{\partial\mathbf{r}}{\partial t}=\mathbf{u}(\mathbf{k})=\frac{1}{\hbar}\nabla_{\mathbf{k}}E(\mathbf{k})\ . \tag{2}$$

The driving force on the electron is $\mathbf{F}=\partial\mathbf{p}/\partial t$ and the final form of Eq. (1) is established.

The overall goal is to study moments of the BTE, Eq. (1), for the case of nonparabolic conduction bands. Thus the first step is to develop a general moment equation. This is achieved by multiplying Eq. (1) by an arbitrary vector (or scalar) operator $\Phi(\mathbf{k})$ and integrating with respect to $\mathbf{k}$ to obtain

$$\int\Phi\frac{\partial f}{\partial t}d^3k+\int\Phi\mathbf{u}\cdot\nabla_{\mathbf{r}}f\,d^3k+\int\Phi\frac{\mathbf{F}}{\hbar}\cdot\nabla_{\mathbf{k}}f\,d^3k=0\ . \tag{3}$$

By noting that Φ is a function of $\mathbf{k}$ alone and invoking the assumption that f approaches zero rapidly enough in the limits of integration such that $\int\nabla_{\mathbf{k}}(\Phi f)d^3k$ is negligible,[46] one obtains the general moment equation

$$\frac{\partial}{\partial t}\int\Phi f\,d^3k=-\nabla_{\mathbf{r}}\cdot\int\Phi\mathbf{u}f\,d^3k+\frac{\mathbf{F}}{\hbar}\cdot\int f\nabla_{\mathbf{k}}\Phi\,d^3k \tag{4}$$

in terms of the driving force $\mathbf{F}$, $\mathbf{k}$-space-dependent electron velocity $\mathbf{u}(\mathbf{k})$, and an arbitrary vector moment operator $\Phi(\mathbf{k})$. Equation (4) represents the mathematical form required to develop the nonparabolic conservation or hydrodynamic transport equations.

For this nonparabolic model, the Kane energy-band dispersion relation[37] for nonparabolic bands will be utilized. This relation is given by

$$\frac{\hbar^2\mathbf{k}^2}{2m^*}=E(\mathbf{k})[1+\alpha E(\mathbf{k})]\ . \tag{5}$$

The specific choice of operators will determine what average physical quantity is conserved in each moment equation. For the first (or zeroth order) moment, let $\Phi_0(\mathbf{k})=1$ in Eq. (4). This gives

$$\frac{\partial}{\partial t}\int f\,d^3k=-\nabla_{\mathbf{r}}\cdot\int\mathbf{u}f\,d^3k\ . \tag{6}$$

This is the familiar continuity equation

$$\frac{\partial n}{\partial t}=-\nabla_{\mathbf{r}}\cdot(n\mathbf{v})\ , \tag{7}$$

where $n=\int f\,d^3k$ is the conduction-band electron density and $\mathbf{v}=(1/n)\int\mathbf{u}f\,d^3k$ is the average electron velocity. The continuity equation is unchanged by the nonparabolic band-structure description.

Traditionally, to generate the second (or first-order)

moment of the BTE, one lets $\Phi_1(\mathbf{k})=\mathbf{p}=\hbar\mathbf{k}$ (or the parabolic band crystal momentum expression $\mathbf{p}$ raised to first order) to develop a conservation-of-momentum equation.[23] However, when considering nonparabolic bands, choosing another factor for the second moment leads to an improved, more compact, mathematical form. This is true primarily due to the eventual need to define the model equations in terms of an average velocity (the full ramifications of this approach will be clearer after the development of the third moment equation). Hence the resulting equation can be manipulated more easily and simplifying approximations can be seen more clearly. Since there is a clearly defined velocity from Eq. (2),

$$\Phi_1(\mathbf{k})=\mathbf{u}(\mathbf{k}) \tag{8}$$

is chosen here as the second moment operator. The use of the nonparabolic velocity $\mathbf{u}(\mathbf{k})$ for the first-order moment operator is a significant improvement in the development of the hydrodynamic transport model. Application of the Kane dispersion relation results in

$$\Phi_1(\mathbf{k})=\mathbf{u}(\mathbf{k})=\frac{\hbar\mathbf{k}}{m(\mathbf{k})} , \tag{9}$$

where from Eq. (5) and the definition for electron velocity

$$m(\mathbf{k})=m^*\left[1+\frac{2\alpha\hbar^2\mathbf{k}^2}{m^*}\right]^{1/2} . \tag{10}$$

Using Eq. (9), $\Phi_1(\mathbf{k})=\mathbf{u}(\mathbf{k})$ in Eq. (4) results in

$$\frac{\partial}{\partial t}\int \mathbf{u}(\mathbf{k})f\,d^3k=-\nabla_r\cdot\int \mathbf{u}(\mathbf{k})\mathbf{u}(\mathbf{k})f\,d^3k + \frac{\mathbf{F}}{\hbar}\cdot\int f\nabla_{\mathbf{k}}\mathbf{u}(\mathbf{k})d^3k . \tag{11}$$

To simplify Eq. (11), consider the last term on the right-hand side. According to previous definitions, the integrand contains the tensor

$$\nabla_{\mathbf{k}}\mathbf{u}(\mathbf{k}) =\frac{\hbar}{m(\mathbf{k})}\begin{bmatrix} 1+\mathcal{A}(\mathbf{k})k_x^2 & \mathcal{A}(\mathbf{k})k_xk_y & \mathcal{A}(\mathbf{k})k_xk_z \\ \mathcal{A}(\mathbf{k})k_yk_x & 1+\mathcal{A}(\mathbf{k})k_y^2 & \mathcal{A}(\mathbf{k})k_yk_z \\ \mathcal{A}(\mathbf{k})k_zk_x & \mathcal{A}(\mathbf{k})k_zk_y & 1+\mathcal{A}(\mathbf{k})k_z^2 \end{bmatrix} , \tag{12}$$

where

$$\mathcal{A}(\mathbf{k})=-\frac{2\alpha\hbar^2}{m^*\left[1+\frac{2\alpha\hbar^2\mathbf{k}^2}{m^*}\right]} . \tag{13}$$

Equation (12) can be written as

$$\nabla_{\mathbf{k}}\mathbf{u}(\mathbf{k})=\frac{\hbar}{m(\mathbf{k})}\left[[\mathbf{I}]+\mathcal{A}(\mathbf{k})\begin{bmatrix} k_x^2 & k_xk_y & k_xk_z \\ k_yk_x & k_y^2 & k_yk_z \\ k_zk_x & k_zk_y & k_z^2 \end{bmatrix}\right] . \tag{14}$$

Any one of the terms in the last matrix of Eq. (14) is of the form $\mathcal{A}(\mathbf{k})k_ik_j$, where i,j can assume any value of the set $\{x,y,z\}$. Therefore, from Eq. (9) these terms may be bounded as

$$|\mathcal{A}(\mathbf{k})k_ik_j| =\frac{2\alpha\hbar^2k_ik_j}{m^*\left[1+\frac{2\alpha\hbar^2\mathbf{k}^2}{m^*}\right]}=2\alpha m^*u_iu_j\le 2\alpha m^*|\mathbf{u}|^2 . \tag{15}$$

For $|\mathbf{u}|=5.0\times10^7$ cm/s, $m^*=0.6\times10^{-31}$ kg, and $\alpha=0.61$ eV^{-1} one has $|\mathcal{A}(\mathbf{k})k_ik_j|\le 0.12$. Clearly, the last matrix in the sum of Eq. (14) represents a higher-order perturbation on the tensor of Eq. (12). Therefore the off-diagonal terms, which would lead to an additional level of complexity, will be neglected and the remaining diagonal terms will be treated to second order in $\mathbf{k}$ to result in the following simplification:

$$\nabla_{\mathbf{k}}\mathbf{u}(\mathbf{k})=\frac{\hbar}{m(\mathbf{k})}[\mathbf{I}] . \tag{16}$$

Using Eq. (16) in Eq. (11) leads to

$$\frac{\mathbf{F}}{\hbar}\cdot\int f\,\nabla_{\mathbf{k}}\mathbf{u}(\mathbf{k})d^3k=\mathbf{F}\int\frac{f}{m(\mathbf{k})}d^3k=n\frac{\mathbf{F}}{\tilde{m}^*} , \tag{17}$$

where

$$\frac{n}{\tilde{m}^*}=\int\frac{f}{m(\mathbf{k})}d^3k . \tag{18}$$

The first term on the right-hand side of Eq. (11) is in the identical form as the parabolic band or classical case and can be manipulated in the same manner[47] to obtain

$$-\nabla_r\cdot\int \mathbf{u}(\mathbf{k})\mathbf{u}(\mathbf{k})f\,d^3k=-\nabla_r\cdot\left[\frac{[\mathbf{P}_v]}{m^*}+n\mathbf{vv}\right] , \tag{19}$$

where $\mathbf{vv}$ is a dyadic product and the effective velocity pressure term is

$$[\mathbf{P}_v]_{i,j}=m^*\int f[u_i(\mathbf{k})-v_i][u_j(\mathbf{k})-v_j]d^3k . \tag{20}$$

However,

$$\nabla_r\cdot(n\mathbf{vv})=\mathbf{v}\nabla_r\cdot(n\mathbf{v})+n\mathbf{v}\cdot\nabla_r\mathbf{v} ; \tag{21}$$

thus

$$-\nabla_r\cdot\int \mathbf{u}(\mathbf{k})\mathbf{u}(\mathbf{k})f\,d^3k =-\nabla_r\cdot\frac{[\mathbf{P}_v]}{m^*}-\mathbf{v}\nabla_r\cdot(n\mathbf{v})-n\mathbf{v}\cdot\nabla_r\mathbf{v} . \tag{22}$$

Expanding the first term on the left-hand side of Eq. (11) yields

$$\frac{\partial}{\partial t}\int \mathbf{u}(\mathbf{k})f\,d^3k=\frac{\partial}{\partial t}(n\mathbf{v})=\mathbf{n}\frac{\partial\mathbf{v}}{\partial t}+\mathbf{v}\frac{\partial n}{\partial t} , \tag{23}$$

which can be combined with Eq. (7), $\partial n/\partial t=-\nabla_r\cdot(n\mathbf{v})$, to obtain

$$\frac{\partial}{\partial t}\int \mathbf{u}(\mathbf{k})f\,d^3k=n\frac{\partial\mathbf{v}}{\partial t}-\mathbf{v}\nabla_r\cdot(n\mathbf{v}) . \tag{24}$$

Combining Eqs. (17), (22), and (24) culminates in the second moment equation given by

$$\frac{\partial \mathbf{v}}{\partial t}=-\mathbf{v}\cdot\nabla_{\mathbf{r}}+\frac{\mathbf{F}}{\tilde{m}^*}-\frac{1}{nm^*}\nabla_{\mathbf{r}}\cdot[\mathbf{P}_{\mathbf{v}}] . \tag{25}$$

The second moment of the BTE given by Eq. (25), which has been derived using the nonparabolic velocity $\mathbf{u}(\mathbf{k})$ and acceptable simplifications, has the identical form to the parabolic or constant effective-mass case,[21,48] with the exceptions that $\tilde{m}^*$ replaces m^* and the definition of $\mathbf{P}_{\mathbf{v}}$ utilizes a more complicated definition of the particle velocity $\mathbf{u}(\mathbf{k})$. As in the parabolic case, additional requirements must be made to simplify $\mathbf{P}_{\mathbf{v}}$ (and $\tilde{m}^*$ for this nonparabolic model) and these will be discussed in Sec. III.

The third (or second-order) moment is usually produced by choosing $\Phi_2(\mathbf{k})=E(\mathbf{k})=(m^*/2)|\mathbf{u}|^2$ (or $2m^*\mathbf{p}^2$ for parabolic bands; thus second order in momentum $\mathbf{p}$) to result in an energy conservation equation. For nonparabolic bands, $E(\mathbf{k})$ is the positive root of $(\hbar^2\mathbf{k}^2)/(2m^*)=E(1+\alpha E)$. This leads to a very troublesome formulation when one attempts to define the moment equations in terms of familiar physical averages. Thus a slightly more transparent path is taken. Energy is chosen as the third moment operator; however, the approximation $E_s(\mathbf{k})\approx E(\mathbf{k})$ is chosen to once again produce an improved mathematical form more conducive to analysis and simplification. The chosen operator is

$$\Phi_2(\mathbf{k})=E_s(\mathbf{k})=\frac{m(\mathbf{k})}{2}\mathbf{u}(\mathbf{k})\cdot\mathbf{u}(\mathbf{k}) , \tag{26}$$

which has a familiar kinetic-energy form $[(m^*/2)\mathbf{u}^2]$ and is second order in $\mathbf{u}(\mathbf{k})$. Before continuing, the error in using this approximation may be bounded by noting that

$$E_s(\mathbf{k})=E(\mathbf{k})\frac{1+\alpha E(\mathbf{k})}{1+2\alpha E(\mathbf{k})} . \tag{27}$$

For a typical value of $\alpha=0.6$ eV^{-1}, Eq. (27) yields $E_s=0.812E$ for $E=0.5$ eV. Therefore this approximation is better than 80% accurate up to energies of 0.5 eV. Figure 1 shows the approximation to the energy for several values of α. The agreement is sufficient for our purposes since above 0.5 eV the Kane dispersion relation does not accurately predict the true band structure.[49]

Using Eq. (26) as an approximate definition of electron energy, the third moment of the BTE becomes

$$\frac{\partial}{\partial t}\int E_s(\mathbf{k})f\,d^3k=-\nabla_{\mathbf{r}}\cdot\int\mathbf{u}(\mathbf{k})E_s(\mathbf{k})f\,^3k + \frac{\mathbf{F}}{\hbar}\cdot\int f\,\nabla_{\mathbf{k}}E_s(\mathbf{k})d^3k . \tag{28}$$

Concentrating on the integrand of the third term one has

$$\nabla_{\mathbf{k}}E_s(\mathbf{k})=\hbar\mathbf{u}(\mathbf{k})[1+\mathcal{B}(\mathbf{k})] , \tag{29}$$

where

$$\mathcal{B}(\mathbf{k})=\frac{-\alpha\hbar^2\mathbf{k}^2}{m^*\left[1+\dfrac{2\alpha\hbar^2\mathbf{k}^2}{m^*}\right]}=\frac{-2\alpha E(\mathbf{k})[1+\alpha E(\mathbf{k})]}{[1+2\alpha E(\mathbf{k})]^2} . \tag{30}$$

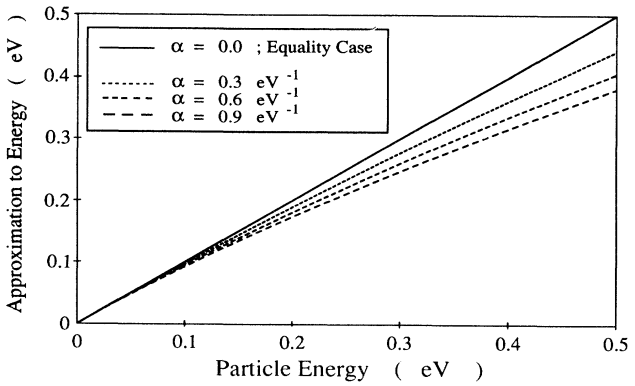

FIG. 1. Evaluation of E_s, the approximation used for the particle energy, vs E for values of conduction-band nonparabolicity parameter.

Thus the last term in Eq. (29) may be bounded by performing an analysis similar to that of Eq. (15). Doing this leads to

$$|\mathcal{B}(\mathbf{k})|=\alpha m^*|\mathbf{u}|^2\le 0.06 \tag{31}$$

for the same set of typical parameter values as before. Therefore, approximating Eq. (29) to third order in $\mathbf{k}$ yields

$$\frac{\mathbf{F}}{\hbar}\cdot\int f\,\nabla_{\mathbf{k}}E_s(\mathbf{k})d^3k=\mathbf{F}\cdot\int\mathbf{u}(\mathbf{k})f\,d^3k=\mathbf{F}\cdot\mathbf{v} . \tag{32}$$

The second term in Eq. (28) can be manipulated in the same manner as the classical or parabolic case[47] to obtain

$$-\nabla_{\mathbf{r}}\cdot\int\mathbf{u}(\mathbf{k})E_s(\mathbf{k})f\,d^3k=-\nabla_{\mathbf{r}}\cdot(\mathbf{v}\cdot[\mathbf{P}_w]+\mathbf{q}) -n\mathbf{v}\cdot\nabla_{\mathbf{r}}w-w\nabla_{\mathbf{r}}\cdot(n\mathbf{v}) . \tag{33}$$

Here the definition $nw=\int E_s(\mathbf{k})f\,d^3k$ has been used as the total average electron kinetic energy, with the approximation $E_s(\mathbf{k})=E(\mathbf{k})$. In Eq. (33), the effective energy pressure term is

$$[\mathbf{P}_{\mathbf{w}}]_{i,j}=\int m(\mathbf{k})[u_i(\mathbf{k})-v_i][u_j(\mathbf{k})-v_j]f\,d^3k \tag{34}$$

and the effective heat-flow vector is

$$\mathbf{q}_i=\int\frac{m(\mathbf{k})}{2}[u_i(\mathbf{k})-v_i][\mathbf{u}(\mathbf{k})-\mathbf{v}]\cdot[\mathbf{u}(\mathbf{k})-\mathbf{v}]f\,d^3k . \tag{35}$$

The first term of Eq. (28) becomes

$$\frac{\partial}{\partial t}\int E_s(\mathbf{k})f\,d^3k=\frac{\partial nw}{\partial t}=n\frac{\partial w}{\partial t}+w\frac{\partial n}{\partial t} , \tag{36}$$

which can be combined with Eq. (7), $\partial n/\partial t=-\nabla_{\mathbf{r}}\cdot(n\mathbf{v})$, to obtain

$$\frac{\partial}{\partial t}\int E_s(\mathbf{k})f\,d^3k=n\frac{\partial w}{\partial t}-w[\nabla_{\mathbf{r}}\cdot(n\mathbf{v})] . \tag{37}$$

Using Eqs. (32), (33), and (37) reduces the third moment equation to

$$\frac{\partial w}{\partial t} = -\mathbf{v}\cdot\nabla_r w + \mathbf{v}\cdot\mathbf{F} - \frac{1}{n}\nabla_r\cdot(\mathbf{v}\cdot[\mathbf{P}_w] + \mathbf{q}) \ . \tag{38}$$

From Eqs. (7), (25), and (38), the nonparabolic hydrodynamic collisionless transport equations for conservation of particles, average momentum, and average energy in Lagrangian form[17] are

$$\frac{\partial n}{\partial t} = -\nabla_r\cdot(n\mathbf{v}) \ , \tag{39}$$

$$\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v}\cdot\nabla_r\mathbf{v} + \frac{\mathbf{F}}{\tilde{m}^*} - \frac{1}{nm^*}\nabla_r\cdot[\mathbf{P}_v] \ , \tag{40}$$

$$\frac{\partial w}{\partial t} = -\mathbf{v}\cdot\nabla_r w + \mathbf{F}\cdot\mathbf{v} - \frac{1}{n}\nabla_r\cdot(\mathbf{v}\cdot[\mathbf{P}_w] + \mathbf{q}) \ , \tag{41}$$

where

$$n = \int f\, d^3k \ , \tag{42}$$

$$n\mathbf{v} = \int \mathbf{u}(\mathbf{k}) f\, d^3k \ , \tag{43}$$

$$nw = \int \frac{m(\mathbf{k})}{2}\mathbf{u}(\mathbf{k})\cdot\mathbf{u}(\mathbf{k}) f\, d^3k \ , \tag{44}$$

$$\frac{n}{\tilde{m}^*} = \int \frac{f}{m(\mathbf{k})} d^3k \ , \tag{45}$$

$$[\mathbf{P}_v] = m^* \int [\mathbf{u}(\mathbf{k}) - \mathbf{v}][\mathbf{u}(\mathbf{k}) - \mathbf{v}] f\, d^3k \ , \tag{46}$$

$$[\mathbf{P}_w] = \int m(\mathbf{k})[\mathbf{u}(\mathbf{k}) - \mathbf{v}][\mathbf{u}(\mathbf{k}) - \mathbf{v}] f\, d^3k \ , \tag{47}$$

$$\mathbf{q} = \int \frac{m(\mathbf{k})}{2}[\mathbf{u}(\mathbf{k}) - \mathbf{v}][\mathbf{u}(\mathbf{k}) - \mathbf{v}]\cdot[\mathbf{u}(\mathbf{k}) - \mathbf{v}] f\, d^3k \ . \tag{48}$$

Before this system of equations can be applied to the study of electron transport additional assumptions must be invoked to express Eqs. (45)–(48) in terms n, $\mathbf{v}$, and w. This mathematical closure entails the use of specific fundamental physical properties to evaluate these parameters. Throughout this section efforts have been made to express these parameters in a mathematical form that is as compact as possible. It is clear that the integral definitions consist primarily of terms involving $\mathbf{u}(\mathbf{k})$ and differ from the definitions for the parabolic case only by the introduction of the nonparabolic mass $m(\mathbf{k})$ and the specific definition of the particle velocity $\mathbf{u}(\mathbf{k})$. This property will be utilized in the following section to develop approximate expressions so that this nonparabolic form of the hydrodynamic equations may be used to study electron dynamics in realistic electronic structures.

III. NONPARABOLIC TRANSPORT MODEL

The preceding equations represent a general nonparabolic hydrodynamic transport model for electron transport in a single valley of GaAs. Additional assumptions or relationships are necessary to close the system of equations before they can be used to describe transport phenomena. Specifically, one must either ignore one or more higher-order terms in the formulation,[21,50] have some previous knowledge for the equations of state,[51,52] or assume some form of the electron distribution function in momentum space.[53] These are all acceptable methods of simplification and can lead to the same unique system of equations.

The use of a predefined distributional form is often viewed as being more restrictive and less general than some of the previous alternatives. Yet many derivations, which seek to develop models applicable for more generalized distributions, partially implement closure relations with properties *proven* true only for specific distributional forms.[9,15] Extending the electron-transport model in this manner has merit and leads to results which are more physically accurate.[9] However, mixing assumptions in this manner can obscure regions of validity for the complete model. Defining a specific form of the distribution function is the most complete approach and easiest to evaluate from both a physical and mathematical point of view. Therefore this is the approach considered here.

The distribution most frequently chosen to describe nonequilibrium transport phenomena is the displaced Maxwellian function. For the case of parabolic conduction bands this distribution function, in momentum space, is[53]

$$f_{\mathrm{DM}}(\mathbf{k}) = \frac{n\hbar^3}{(2\pi m^* k_B T_e)^{3/2}} \exp\left[\frac{-\hbar^2|\mathbf{k}-\mathbf{k}_d|^2}{2m^* k_B T_e}\right] \ , \tag{49}$$

where k_B is the Boltzmann constant, T_e is the temperature of the electron gas representing the spread of the distribution, and $\mathbf{k}_d$ is the displacement from $\mathbf{k}=0$ of the Maxwellian distribution. The previous distribution ignores any effect that Fermi-Dirac statistics may have on the total number of available electrons. Since this work is directed toward transport in conduction bands and it is a simple task to modify the normalization coefficient to include these Fermi effects they will be ignored throughout. This Maxwellian approach[10] has been applied often in the analysis of such problems; however, for the case of nonparabolic bands Monte Carlo calculations indicate that such a distribution leads to a less than adequate treatment of the transport parameters of the hydrodynamic model.[39]

In this derivation a unique treatment is proposed for closing the general moment equations for electron transport in GaAs. To articulate the basis of this approach, consider a form of the displaced Maxwellian distribution $\mathcal{F}_{\mathrm{DM}}(\mathbf{u})$ transformed into velocity space such that $\mathcal{F}_{\mathrm{DM}}(\mathbf{u})d^3u = f_{\mathrm{DM}}(\mathbf{k})d^3k$ or, specifically, $\mathcal{F}_{\mathrm{DM}}(\mathbf{u}) = |J_{\mathrm{DM}}| f(\mathbf{u}^{-1}(\mathbf{k}))$. Here the inverse function $\mathbf{u}^{-1}(\mathbf{k})$ represents the function $\mathbf{u}^{-1}(\mathbf{k}) = \mathbf{k} = \mathbf{g}(\mathbf{u})$ where $\mathbf{g}(\mathbf{u})$ is the correct mapping from momentum space to velocity space. Also, J_{DM} is the appropriate Jacobian transformation[54] from momentum space to velocity space. Defining this velocity space distribution in such a manner allows parametric definitions of the form $I = \int i(\mathbf{k}) f_{\mathrm{DM}}(\mathbf{k}) d^3k$, similar to Eqs. (45)–(48), to be expressed in velocity space as $I = \int i(\mathbf{u}^{-1}(\mathbf{k}))\mathcal{F}_{\mathrm{DM}}(\mathbf{u}) d^3u$. Therefore, for the case of parabolic bands where the relationship between velocity space and momentum space is linear, $\mathbf{u}(\mathbf{k}) = (\hbar\mathbf{k})/m^*$ and $|J_{\mathrm{DM}}| = (m^*/\hbar)^3$, this corresponding displaced Maxwellian distribution in velocity space is

$$\mathcal{F}_{\mathrm{DM}}(\mathbf{u})=n\left[\frac{m^*}{2\pi k_B T_e}\right]^{3/2}\exp\left[\frac{-m^*|\mathbf{u}-\mathbf{v}|^2}{2k_B T_e}\right], \tag{50}$$

where $\mathbf{v}$ now represents the average velocity as well as the displacement under consideration in velocity space. Both Eqs. (49) and (50) are symmetric about their displacements within their respective spaces and the average velocity $\mathbf{v}$ is equal to $(\hbar\mathbf{k}_d)/m^*$; therefore Eq. (50) does represent a completely consistent transformation of Eq. (49) for the case of parabolic bands.

One would expect that, under the conditions of nonparabolic bands where the effective mass of the electron depends on the precise location in the conduction band, the use of constant m^* would be insufficient. Also, another dilemma exists in defining a single temperature of the electron gas since it has been shown that two distinctly different temperatures tensors $\mathbf{T}_v$ and $\mathbf{T}_w$ occur for the case of nonparabolic bands.[39] Thus stationary Monte Carlo calculations and physical intuition suggests the following ansatz distribution:

$$\mathcal{F}_{\mathrm{nonpar}}(\mathbf{u})=n\left[\frac{m_w(\mathbf{v},T_w)}{2\pi k_B T_w}\right]^{3/2}\times\exp\left[\frac{-m_w(\mathbf{v},T_w)|\mathbf{u}-\mathbf{v}|^2}{2k_B T_w}\right] \tag{51}$$

as a constitutive relation to close the moment equations for the case of nonparabolic energy bands. Here a single effective temperature T_w is still utilized. However, T_w, with a distinct w subscript, has been chosen to replace T_e because $\frac{3}{2}k_B T_w$ (here T_w is defined from diagonal elements of the energy pressure $[\mathbf{P}_w]$) approximates the effective thermal energy well for the stationary transport case at moderate values of average energy.[39] In addition, $m_w(\mathbf{v},T_w)$ has been introduced because, based on physical considerations, we expect a nonconstant average effective mass which should depend strongly on the spread or thermal component T_w of the true electron distribution and on the displacement in velocity space $\mathbf{v}$.

In applying Eq. (51) to the integral definitions (42)–(48), it is correct to use $\mathcal{F}_{\mathrm{nonpar}}(\mathbf{u})d^3u=f_{\mathrm{nonpar}}(\mathbf{k})d^3k$, since $\mathcal{F}_{\mathrm{nonpar}}$ was postulated in velocity space from a distribution which contained this transformation property. However, the issue of transformating between momentum and velocity space for the case of nonparabolic bands involves very complicated nonlinear transformations. Thus it is instructive to consider this issue briefly. Assume for the moment that a correct form for the distribution in momentum space is known and denote this distribution as $f_{\mathrm{nonpar}}(\mathbf{k})$. To preserve the property $\mathcal{F}_{\mathrm{nonpar}}(\mathbf{u})d^3u=f_{\mathrm{nonpar}}(\mathbf{k})d^3k$ so that transforming integral definitions consists just of inverting the $i(\mathbf{k})$ in $I=\int i(\mathbf{k})f_{\mathrm{DM}}(\mathbf{k})d^3k$, a new nonlinear transformation factor J_{nonpar}, such that

$$\mathcal{F}_{\mathrm{nonpar}}(\mathbf{u})=|J_{\mathrm{nonpar}}|f_{\mathrm{nonpar}}(\mathbf{u}^{-1}(\mathbf{k})), \tag{52}$$

is needed. In Eq. (52), $\mathbf{u}^{-1}(\mathbf{k})=\mathbf{k}=\mathbf{g}(\mathbf{u})$ is assumed to exist and to be a single-valued function of $\mathbf{u}$. This can be shown to be true for transformations from a finite region about $\mathbf{k}=0$ in momentum space to a finite region about $\mathbf{u}=0$ in velocity space.[55]

For the case of nonparabolic bands, defined by relation (5) and a resulting nonlinear momentum space velocity $\mathbf{u}(\mathbf{k})$ given by Eq. (9), the appropriate factor is $J_{\mathrm{nonpar}}=j_{\mathrm{nonpar}}$ where[54]

$$j_{\mathrm{nonpar}}=\begin{vmatrix}\frac{\partial u_x}{\partial k_x}&\frac{\partial u_x}{\partial k_y}&\frac{\partial u_x}{\partial k_z}\\ \frac{\partial u_y}{\partial k_x}&\frac{\partial u_y}{\partial k_y}&\frac{\partial u_y}{\partial k_x}\\ \frac{\partial u_x}{\partial k_x}&\frac{\partial u_x}{\partial k_y}&\frac{\partial u_x}{\partial k_z}\end{vmatrix}. \tag{53}$$

Using the definition of $\mathbf{u}(\mathbf{k})$ given by Eq. (9) in Eq. (53) results in

$$j_{\mathrm{nonpar}}=\left[\frac{\hbar}{m(\mathbf{k})}\right]^3\begin{vmatrix}1+\mathcal{C}(\mathbf{k})k_x^2&\mathcal{C}(\mathbf{k})k_xk_y&\mathcal{C}(\mathbf{k})k_xk_z\\ \mathcal{C}(\mathbf{k})k_yk_x&1+\mathcal{C}(\mathbf{k})k_y^2&\mathcal{C}(\mathbf{k})k_yk_z\\ \mathcal{C}(\mathbf{k})k_zk_x&\mathcal{C}(\mathbf{k})k_zk_y&1+\mathcal{C}(\mathbf{k})k_z^2\end{vmatrix}, \tag{54}$$

where

$$\mathcal{C}(\mathbf{k})=-\frac{2\alpha\hbar^2}{m^*\left[1+\frac{2\alpha\hbar^2\mathbf{k}^2}{m^*}\right]}. \tag{55}$$

The transform defined by Eq. (54) is extremely complex. Also, it is obvious that completing the remaining determinate operation and performing the necessary functional substitution will introduce cross-coupled real-space transformation factors. Therefore, to gain more insight in this investigation, the near equilibrium case will be considered where most of the electrons are near the conduction-band minimum. For this case the off-diagonal terms may be neglected and Eq. (54) can be approximated to lowest order in $\mathbf{k}$ to obtain

$$j_{\mathrm{nonpar}}=\left[\frac{\hbar}{m(\mathbf{u}^{-1}(\mathbf{k}))}\right]^3. \tag{56}$$

In order to proceed further more information about the distribution in momentum space appropriate for nonparabolic bands is necessary. The concept of a Maxwellian function,[56] where the distribution assumed is of the form $(n/I_n)\exp[-E(\mathbf{k})/(k_B T_e)]$ (where I_n is the appropriate normalization factor), will now be applied to generate a test distribution in momentum space to gain additional insight. Doing this and using the approximate definition for electron energy from Eq. (26) results in a simplified illustrative distribution, under displacement $\mathbf{k}_d$, of

$$f_{\text{nonpar}}(\mathbf{k})=\frac{n}{I_n}\exp\left[\frac{-m(\mathbf{k}-\mathbf{k}_d)\mathbf{u}^2(\mathbf{k}-\mathbf{k}_d)}{2k_BT_e}\right]. \quad (57)$$

Using Eq. (57) as a test function, the transformation Eq. (52) yields

$$\mathcal{F}_{\text{nonpar}}(\mathbf{u})=\frac{n}{I_n}\left[\frac{m(\mathbf{u}^{-1}(\mathbf{k}))}{\hbar}\right]^3\times\exp\left[\frac{-m(\mathbf{u}_v^{-1}(\mathbf{k}-\mathbf{k}_d))\mathbf{u}^2(\mathbf{u}_v^{-1}(\mathbf{k}-\mathbf{k}_d))}{2k_BT_e}\right], \quad (58)$$

where for this distribution $\mathbf{u}^{-1}(\mathbf{k})$ represents the function $\mathbf{u}^{-1}(\mathbf{k})=\mathbf{k}=\mathbf{g}(\mathbf{u})$ and $\mathbf{u}_v^{-1}(\mathbf{k})$ represents some undefined function of the form $\mathbf{u}_v^{-1}(\mathbf{k})=\mathbf{k}-\mathbf{k}_d=\mathbf{g}(\mathbf{u}-\mathbf{v})$.

Examination of Eq. (58) reveals that the exponential argument is modulated by a function $m(\mathbf{u}_v^{-1}(\mathbf{k}-\mathbf{k}_d))$, which resembles an effective-mass term with velocity displacement dependence. Also, the effective normalization function contains an effective-mass term which has velocity dependence. The simplified $\mathcal{F}_{\text{nonpar}}$ derived here does not exhibit the exact form of the ansatz distribution function defined by Eq. (51). However, the previous analysis does lend theoretical support to the idea of using the intuitively derived $\mathcal{F}_{\text{nonpar}}$ of Eq. (51) as a tool to investigate nonequilibrium electron transport for the case of nonparabolic conduction bands. Indeed, later it will be shown that this distribution leads to excellent results for nonequilibrium transport in nonparabolic conduction bands.

Now that the basis of the $\mathcal{F}_{\text{nonpar}}(\mathbf{u})$ distribution function, Eq. (51), has been considered through a simplified but rigorous analysis, some of its properties will be presented before proceeding. The distribution is symmetric in velocity space about a displacement of the average velocity $\mathbf{v}$. Though the spread in velocity space is symmetric, the amount of spread depends in a nonlinear way on temperature T_w and displacement $\mathbf{v}$. Specifically, the dependence of the spread is partially determined by the free function $m_w(\mathbf{v},T_w)$. This distribution *does* meet the expected and necessary requirements of yielding the average electron density n upon evaluation of $\int\mathcal{F}_{\text{nonpar}}d^3u$ and the average electron velocity $\mathbf{v}$ upon evaluating $(1/n)\int\mathbf{u}\mathcal{F}_{\text{nonpar}}d^3u$. Also, $\mathcal{F}_{\text{nonpar}}(\mathbf{u})$ converges to $\mathcal{F}_{\text{DM}}(\mathbf{u})$ as $m_w\rightarrow m^*$. This last quality is desirable because the Maxwellian-based distribution $\mathcal{F}_{\text{DM}}(\mathbf{u})$ is considered to be a good approximation for the case of small perturbations from equilibrium and dominate electron-electron scattering.[57]

At this point the first question to address is how to define $m_w(\mathbf{v},T_w)$. One way would be to study either experimentally obtained or Monte Carlo–generated electron distributions in velocity space. However, since the postulation and inclusion of $m_w(\mathbf{v},T_w)$ in the distribution function was based on the idea of a nonconstant effective mass, a more interesting approach is to approximate $m_w(\mathbf{v},T_w)$ by average effective mass of the entire distribution. Equating $m_w(\mathbf{v},T_w)$ to the definition of the inverse average effective mass of Eq. (45),

$$\tilde{m}^*=\left[\frac{1}{n}\int\frac{\mathcal{F}_{\text{nonpar}}}{m(\mathbf{u}^{-1}(\mathbf{k}))}d^3u\right]^{-1} \quad (59)$$

yields the recursive definition

$$m_w(\mathbf{v},T_w)=\left[\left[\frac{m_w(\mathbf{v},T_w)}{2\pi k_BT_w}\right]^{3/2}\times\int\frac{\exp\left[\frac{-m_w(v,T_w)|\mathbf{u}-\mathbf{v}|^2}{2k_BT_w}\right]}{m(\mathbf{u}^{-1}(\mathbf{k}))}d^3u\right]^{-1}. \quad (60)$$

Here $m(\mathbf{u}^{-1}(\mathbf{k}))$ is defined using Eqs. (10) and (9), which to fourth order in $\mathbf{u}$ become

$$\frac{1}{m(\mathbf{u}^{-1}(\mathbf{k}))}=\frac{1}{m^*}\left[1-\alpha m^*|\mathbf{u}|^2-\frac{\alpha^2}{2}(m^*)^2|\mathbf{u}|^4\right]. \quad (61)$$

The above formulation has been written in terms of velocity to simplify the integration process required here and later in the paper. Performing the integration in Eq. (60) results in the approximate expression of

$$m_w(\mathbf{v},T_w)=m^*(1+3\alpha k_BT_w+7.5(\alpha k_BT_w)^2+\alpha m^*|\mathbf{v}|^2). \quad (62)$$

The preceding formula resulted from the recursive definition of Eq. (60) and the method of defining $m_w(\mathbf{v},T_w)$ merits further investigation. Within the framework of this nonparabolic model $m_w(\mathbf{v},T_w)$ is a free parameter which one may arbitrarily choose. Consider the simple definition of

$$m_w(\mathbf{v},T_w)=m^*(1+\mathcal{A}_w\alpha k_BT_w+\mathcal{B}_w\alpha m^*|\mathbf{v}|^2), \quad (63)$$

where the result from Eq. (62) has been used to define an effective normalized lower-order form for $m_w(\mathbf{v},T_w)$ with $\mathcal{A}_w$ and $\mathcal{B}_w$ as fitting parameters. Using (63) in the definition for $\tilde{m}^*$ results in the approximate formula

$$\tilde{m}^*(\mathbf{v},T_w)=m^*(1+3\alpha k_BT_w+(7.5-3\mathcal{A}_w)(\alpha k_BT_w)^2+\alpha m^*|\mathbf{v}|^2). \quad (64)$$

From this result one can observe that the first-order result for $\tilde{m}^*$ is independent of the definition of $m_w(\mathbf{v},T_w)$ and represents a perturbational effect on the second-order terms in T_w (here higher-order terms have been excluded, hence the disappearance of $\mathcal{B}_w$). Also, since

$$(1/n)\int m(\mathbf{u}^{-1}(\mathbf{k}))\mathcal{F}_{\text{nonpar}}d^3u\approx\left[(1/n)\int\mathcal{F}_{\text{nonpar}}/m(\mathbf{u}^{-1}(\mathbf{k}))d^3u\right]^{-1},$$

to second order in T_w and $\mathbf{u}$, the last derivation has also resulted in an approximate expression for the transport parameter

$$\tilde{m}^*_{\rm av}=(1/n)\int m(u^{-1}(\mathbf{k}))\mathcal{F}_{\rm nonpar}d^3u$$

(this parameter will be required later in the derivation). Hence, throughout this work the definitions

$$\tilde{m}^*(\mathbf{v},T_w)=\tilde{m}^*_{\rm av}(\mathbf{v},T_w)=m_w(\mathbf{v},T_w) \tag{65}$$

will be utilized.

Combining the proposed distribution of Eq. (51) with the preceding result supplies the complete constitutive relation to close the moment equations of Sec. II. Applying these relations to the energy pressure tensor $[\mathbf{P}_w]$ results in

$$[\mathbf{P}_w]=nk_BT_w\mathcal{T}(\mathbf{v},T_w)[\mathbf{I}]\ , \tag{66}$$

where

$$\mathcal{T}(\mathbf{v},T_w)=\frac{m^*}{\tilde{m}^*}\left[1+2\alpha m^*|\mathbf{v}|^2+5\alpha\frac{m^*}{\tilde{m}^*}k_BT_w+\cdots\right]. \tag{67}$$

Approximating $\mathcal{T}(\mathbf{v},T_w)$ to second order in $\mathbf{v}$ and T_w without cross terms yields a simplified form of

$$\mathcal{T}(\mathbf{v},T_w)=(1+2\alpha k_BT_w+\alpha m^*|\mathbf{v}|^2) \tag{68}$$

and an energy pressure tensor of

$$[\mathbf{P}_w]=nk_BT_w(1+2\alpha k_BT_w+\alpha m^*|\mathbf{v}|^2)[\mathbf{I}]\ . \tag{69}$$

Again applying Eq. (51) and the definition for the average distributional mass to the velocity pressure tensor $[\mathbf{P}_v]$ yields

$$[\mathbf{P}_v]=\frac{m^*}{\tilde{m}^*}nk_BT_w[\mathbf{I}]\ . \tag{70}$$

Using the same approach on the definition of heat-flow vector $\mathbf{q}$ results in

$$\mathbf{q}=5\alpha\left[\frac{m^*}{\tilde{m}^*}\right]^2(k_BT_w)^2\left[1+21\alpha\frac{m^*}{\tilde{m}^*}k_BT_w\right]n\mathbf{v}\ . \tag{71}$$

A relation can now be developed to eliminate T_w from the formulation by studying

$$\frac{1}{n}\int\frac{m(\mathbf{u}^{-1}(\mathbf{k}))}{2}|\mathbf{u}-\mathbf{v}|^2\mathcal{F}_{\rm nonpar}d^3u\ , \tag{72}$$

which is the expression used to define the classical temperature of a gas except with $m(\mathbf{u}^{-1}(\mathbf{k}))=$const. Performing the same integration steps as used to simplify the energy pressure tensor results in

$$\tfrac{3}{2}k_BT_w\mathcal{T}(\mathbf{v},T_w)=\frac{1}{n}\int\frac{m(\mathbf{u}^{-1}(\mathbf{k}))}{2}|\mathbf{u}-\mathbf{v}|^2f\,d^3u\ . \tag{73}$$

The preceding expression can also be expanded to yield

$$\frac{1}{n}\int\frac{m(\mathbf{u}^{-1}(\mathbf{k}))}{2}|\mathbf{u}-\mathbf{v}|^2f\,d^3u=w+\frac{\tilde{m}^*}{2}\mathbf{v}\cdot\mathbf{v}-\tilde{m}^*_{\rm au}\mathbf{v}\cdot\mathbf{v} \tag{74}$$

to second order in $\mathbf{v}$ and T_w. Using the definition of Eq. (65) leads to the final constitutive relation

$$w=\tfrac{3}{2}k_BT_{\rm eff}(\mathbf{v},T_w)+\frac{\tilde{m}^*(\mathbf{v},T_w)}{2}|\mathbf{v}|^2 \tag{75}$$

with $T_{\rm eff}(\mathbf{v},T_w)=T_w\mathcal{T}(\mathbf{v},T_w)$.

Equation (75) is a nonparabolic form relating the average energy of the electron gas to its effective thermal and kinetic-energy components. It is interesting that this equation is identical to the classical case except $T_{\rm eff}$ replaces T_e and $\tilde{m}^*$ is substituted for the constant mass m^*. This equation, as stated earlier, provides the final relation necessary to close the general moment equations. To summarize the previous developments of this section, the following equations:

$$\tilde{m}^*(\mathbf{v},T_w)=m^*[1+3\alpha k_BT_w+7.5(\alpha k_BT_w)^2+\alpha m^*|\mathbf{v}|^2]\ , \tag{76}$$

$$[\mathbf{P}_v]=\frac{m^*}{\tilde{m}^*}nk_BT_w[\mathbf{I}]\ , \tag{77}$$

$$[\mathbf{P}_w]=nk_BT_w(1+2\alpha k_BT_w+\alpha m^*|\mathbf{v}|^2)[\mathbf{I}]\ , \tag{78}$$

$$\mathbf{q}=5\alpha\left[\frac{m^*}{\tilde{m}^*}\right]^2(k_BT_w)^2\left[1+21\alpha\frac{m^*}{\tilde{m}^*}k_BT_w\right]n\mathbf{v}\ , \tag{79}$$

along with the rearranged form of Eq. (75)

$$T_w=\frac{2}{3k_B}\left[w-\frac{m^*}{2}|\mathbf{v}|^2\right]\left[\frac{1-\frac{4}{3}\alpha w}{1+\alpha m^*|\mathbf{v}|^2}\right] \tag{80}$$

supply all that is necessary to express the hydrodynamic transport model for nonparabolic conduction bands in terms of the quantities: electron concentration n, average electron velocity $\mathbf{v}$, average electron energy w, and the space-time variable $(\mathbf{r},t)$. Applying the preceding relations reveals the collisionless nonparabolic hydrodynamic transport model equations to be

$$\frac{\partial n}{\partial t}=-\nabla_{\mathbf{r}}\cdot(n\mathbf{v})\ , \tag{81}$$

$$\frac{\partial\mathbf{v}}{\partial t}=-\mathbf{v}\cdot\nabla_{\mathbf{r}}\mathbf{v}+\frac{\mathbf{F}}{m^*\mu}-\frac{2}{3nm^*}\nabla_{\mathbf{r}}[n\nu(w-\tfrac{1}{2}m^*|\mathbf{v}|^2)]\ , \tag{82}$$

$$\frac{\partial w}{\partial t}=-\mathbf{v}\cdot\nabla_{\mathbf{r}}w+\mathbf{F}\cdot\mathbf{v}-\frac{2}{3n}\nabla_{\mathbf{r}}\cdot[n\mathbf{v}(\omega=\varphi)(w-\tfrac{1}{2}m^*|\mathbf{v}|^2)], \tag{83}$$

with nonparabolic correction terms

$$\mu(\mathbf{v},w)=1+2\alpha\epsilon(\mathbf{v},w)(w-\tfrac{1}{2}m^*|\mathbf{v}|^2)+\frac{10\alpha^2}{3}[\epsilon(\mathbf{v},w)]^2(w-\tfrac{1}{2}m^*|\mathbf{v}|^2)^2+\alpha m^*|\mathbf{v}|^2\ , \tag{84}$$

$$\nu(\mathbf{v},w)=\frac{\epsilon(\mathbf{v},w)}{\mu(\mathbf{v},w)}\ , \tag{85}$$

$$\omega(\mathbf{v},w)=\epsilon(\mathbf{v},w)[1+\tfrac{4}{3}\alpha\epsilon(\mathbf{v},w)(w-\tfrac{1}{2}m^*|\mathbf{v}|^2)+\alpha m^*|\mathbf{v}|^2]\ , \tag{86}$$

$$\varphi(\mathbf{v},w)=\frac{10\alpha}{3}[\nu(\mathbf{v},w)]^2(\omega-\tfrac{1}{2}m^*\mathbf{v}\cdot\mathbf{v})\times[1+14\alpha\nu(\mathbf{v},w)(w-\tfrac{1}{2}m^*\mathbf{v}\cdot\mathbf{v})]\ , \tag{87}$$

where

$$\epsilon(\mathbf{v},w)=\frac{1-\frac{4}{3}\alpha w}{1+\alpha m^*|\mathbf{v}|^2} \quad (88)$$

The nonparabolic model equations above have been written in a form so that for the parabolic case $\alpha=0$, it is easy to observe that $\mu=\nu=\omega=1$ and $\varphi=0$. Then the nonparabolic model conveniently reduces to the more familiar classical hydrodynamic equations in Lagrangian form.

IV. TRANSPORT MODEL PARAMETER EVALUATION

The nonparabolic hydrodynamic model derived in Sec. III ignored any specific form of scattering mechanisms. This was done primarily to simplify the analysis and to allow for a clear focus on the transport parameters which evolve from the collisionless BTE for nonparabolic bands. To evaluate the results of the preceding section one could assume a form for the scattering mechanism and then solve the resulting system of equations with appropriate boundary conditions (several of the present authors have performed such a study[58]). Results for electron current could then be used to judge the macroscopic feasibility of the nonparabolic model. However, the issue of choosing accurate forms for scattering terms is a complicated one and the specific form has a large influence on the results obtained. Therefore a different initial approach will be followed. The specific approach will be to calculate the resultant nonparabolic parameters $\tilde{m}^*$, $[\mathbf{P}_v]$, $[\mathbf{P}_w]$, and $\mathbf{q}$ of the hydrodynamic model for various structures using an elaborate Monte Carlo model. Since the results of Sec. IV presented formulas for each of the model parameters in terms of average velocity $\mathbf{v}$ and average energy w, the values predicted by these formulas can easily be compared to those from the more elaborate and detailed Monte Carlo model. Taking this approach will give an excellent gauge of the accuracy of the terms of the model without the possible errors introduced by using incorrect forms for the loss mechanisms.

The first test applied was to generate the electron distribution and nonparabolic parameters, directly from their integral definitions (45)–(48), for a time steady-state constant field structure over a variety of electric-field values using Monte Carlo techniques. For these stationary investigations, two independent Monte Carlo models[42,43] were used to analyze electron transport in GaAs. Both of these models utilize single-particle Monte Carlo procedures to improve computational accuracy and efficiency. The models incorporate three valley analytical band structures and included all the significant scattering mechanisms with polar optical intervalley scattering. In addition, both models used the same material and physical parameters.[59]

Under these stationary conditions, as can be observed directly from Eqs. (39)–(41) or indirectly in Eqs. (81)–(83), only the value of $\tilde{m}^*$ will affect the final solution for transport. This is true because all the other terms are space differential in nature. However, as will be shown, these terms do have finite values which vary widely over the cases considered. Also, for these conditions, all the displacement terms (terms of form $\alpha m^*|\mathbf{v}|^2$) in Eqs. (76)–(79) are found to be negligible. Hence this is an excellent test for the accuracy of the derived nonparabolic model parameters and their dependence on energy temperature T_w. The test also reveals how well T_w is determined by its dependence on total kinetic energy w and the displacement kinetic-energy term $(m^*/2)|\mathbf{v}|^2$ via Eq. (80). An investigation into the true electron distribution is also very important since $\mathcal{F}_{\text{nonpar}}$ is instrumental in determining the final formulas for the nonparabolic terms.

The results of these stationary investigations, with the two independent Monte Carlo models in agreement, are presented in Figs. 2–5. Figure 2 exhibits the resulting Monte Carlo generated distribution, the ansatz distribution $\mathcal{F}_{\text{nonpar}}$, and the displaced Maxwellian distribution $\mathcal{F}_{\text{DM}}$ along the direction of applied field, in velocity space, for two values of electric field. Here the Monte Carlo distributions were obtained by sampling electrons in a different velocity volume element from the three-dimensional velocity space. In the calculations, a limiting velocity v_s is used to define the size of the element in the directions other than that of the electric field. Also, v_s was chosen small enough to clearly and accurately show the velocity distribution and large enough for practical simulation time.

Figure 2 clearly indicates that the corrected electron distribution $\mathcal{F}_{\text{nonpar}}$ is a distinct improvement over the displaced Maxwellian. Using $\mathcal{F}_{\text{DM}}$ results in a general tendency, for any select average velocity and energy, to overspread and place too many electrons in the tail of the distribution. Conversely, the improved distribution $\mathcal{F}_{\text{nonpar}}$ retains more electrons closer to equilibrium. This result seems correct for the situation of an energy-dependent effective particle mass (or nonparabolic conduction band) and is verified by the Monte Carlo generated distribution.

The stationary results for a variety of electric-field values, corresponding to the nonparabolic transport pa-

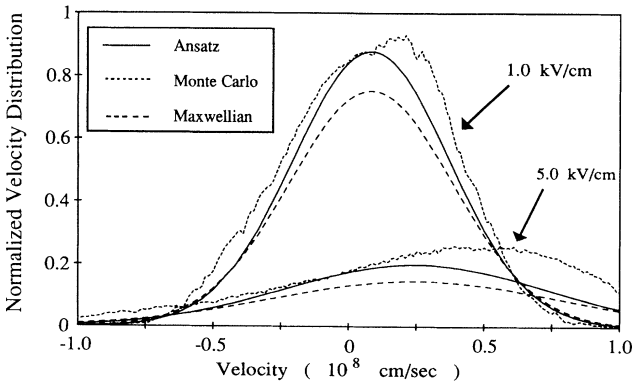

FIG. 2. Normalized Γ-valley velocity distribution functions resulting from the constant electric-field values of 1.0 and 5.0 kV/cm. The profiles are exhibited along the direction of net average velocity (along direction of applied field). All distributions shown are consistently normalized to contain an identical number of electrons.

rameters, are presented in Figs. 3–5 and are plotted versus the average electron energy for each case. In each instance, the nonparabolic transport parameters predicted by the hydrodynamic model were calculated using the Monte Carlo values for average velocity **v** and average energy w since they are fundamentally dependent on these variables.

In general, the predictions supplied by the nonparabolic parameter formulas are in excellent agreement with the results calculated by the Monte Carlo model. Figure 3 shows that the values for the average effective mass $\tilde{m}^*$ predicted by the hydrodynamic model are essentially equal (less than 1% difference) to those calculated by the Monte Carlo model up to 0.4 eV. Figure 4, which gives both the momentum pressure [$\mathbf{P}_v$] and the energy pressure [$\mathbf{P}_w$], clearly shows that these tensors are approximated well by a diagonal matrix. Furthermore, the diagonal elements for both are in very good agreement with the predictions made by the hydrodynamic model. Finally, Fig. 5 shows the comparison between the hydrodynamic model's values for the heat-flow vector **q** and those calculated by Monte Carlo. These results also agree very well, which leads to a very important conclusion. The nonzero expression for the heat-flow vector was derived here from first principles for the nonparabolic conduction-band case. This treatment represents an original *nonequilibrium analysis* for the heat-flow vector which is usually based upon equilibrium thermodynamics arguments. However, it should also be noted that for highly nonstationary conditions this term may need to be determined by higher moments of the BTE before it is accurate for transport simulations.[60]

While the previous stationary results are very positive, by themselves they are not sufficient to ensure the applicability of the present model to arbitrary electron-device structures. Realistic device structures, operating under moderately high biases, always contain regions where transport occurs under nonstationary conditions. Hence additional calculations were performed to determine the accuracy of the nonparabolic model subject to these conditions. The n^+-n-n^+ ballistic diode, a simple prototype submicrometer structure which has been extensively studied,[61] was chosen as a test device.

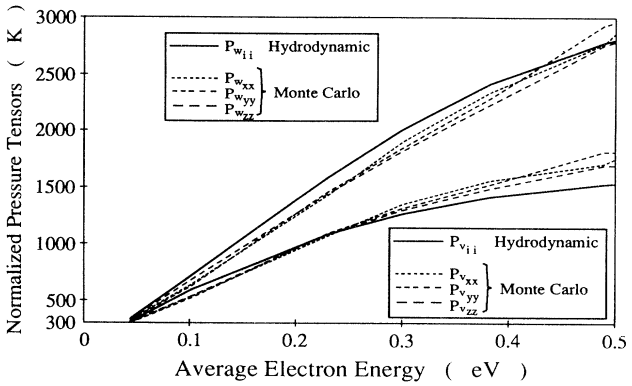

FIG. 4. Velocity and energy Γ-valley pressure tensors, normalized by nk_B, vs average electron energy. The off-diagonal terms are omitted because they are negligible (an order of magnitude smaller) compared to diagonal terms. These results were calculated for stationary transport conditions.

A self-consistent ensemble Monte Carlo model[43] was used to calculate the nonparabolic parameters for several strategically selected locations within this device as illustrated in Fig. 6. Specifically, locations were selected which would exhibit different types of nonstationary transport. At location (1) the electron gas is relatively cool with a low average energy, while the average velocity is slightly ballistic. Conversely, at location (3) the average energy remains high and the average velocity is low. Finally, location (2) represents a case where both gas parameters are elevated and are experiencing significant spatial gradients.

The results of these nonstationary studies are presented in Figs. 7–10 where the various transport parameters are plotted as a function of applied bias. Summarizing the results, the transport parameters predicted by the hydro-

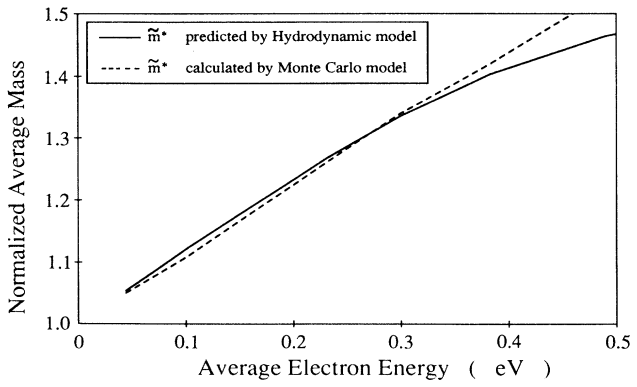

FIG. 3. Average Γ-valley effective mass $\tilde{m}^*$ normalized by near-equilibrium mass value of $m^* = 0.57 \times 10^{-21}$ kg and plotted vs average electron energy w. These results were calculated for stationary transport conditions.

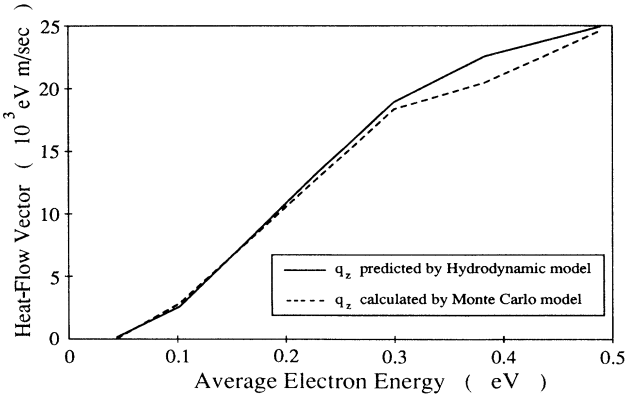

FIG. 5. Γ-valley heat-flow vector along the direction of applied electric field, normalized by n, vs average electron energy. The other vector components are omitted because they are negligible compared to field direction component. These results were calculated for stationary transport conditions.

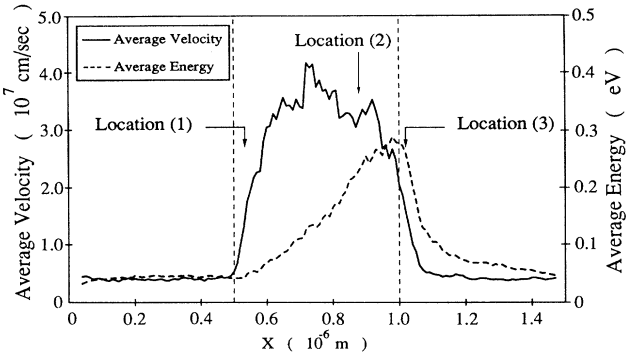

FIG. 6. Γ-valley average velocity and energy profiles through a submicrometer GaAs n^+-n-n^+ ballistic diode structure biased at 0.8 V. The structure consists of 0.5-μm-long source and collector regions doped 10^{17} cm^{-3} with a 0.5-μm active region doped 10^{16} cm^{-3}. The diagram also indicates three locations ($x=0.53$, 0.85, and 1.03 μm) where the nonparabolic model transport parameters were investigated using the Monte Carlo method.

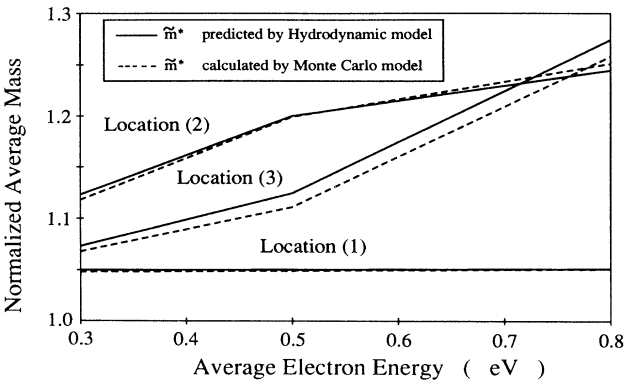

FIG. 7. Normalized average Γ-valley effective mass, at three locations within the ballistic diode, plotted as a function of applied bias.

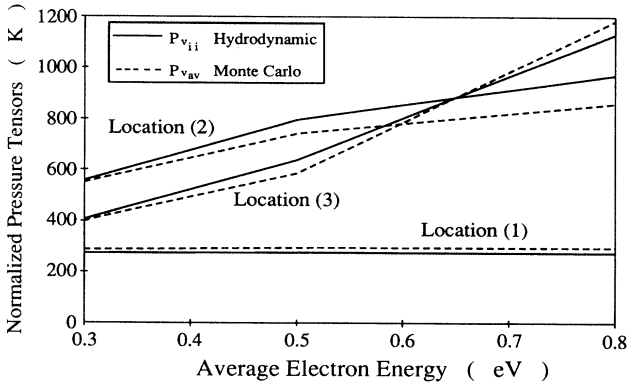

FIG. 8. Normalized Γ-valley velocity pressure, at three locations within the ballistic diode, plotted as a function of applied bias. $P_{v_{av}}$ represents the average of the three diagonal components which were found from Monte Carlo calculations to be approximately equal. Off-diagonal terms were negligibly small.

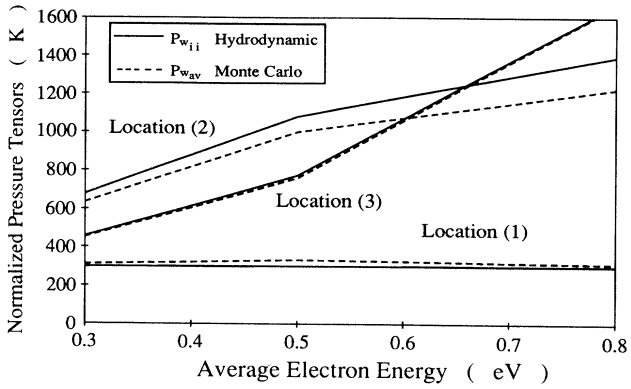

FIG. 9. Normalized Γ-valley energy pressure, at three locations within the ballistic diode, plotted as a function of applied bias. $P_{w_{av}}$ represents the average of the three diagonal components which were found from Monte Carlo calculations to be approximately equal. Off-diagonal terms were negligibly small.

dynamic model are in very good agreement with the direct Monte Carlo calculations. In fact, the agreement for all parameters is within 10% for the majority of the biases studied. In fact, the difference only rises slightly higher to approximately 20% (for the heat-flow vector) at low biases where the accuracy of the Monte Carlo statistics is in question. The results agreed both qualitatively and quantitatively for all three locations and at all biases. Hence all the results indicate this nonparabolic hydrodynamic model can accurately approximate electron transport in realistic semiconductor devices which exhibit nonlocal electron transport effects.

V. CONCLUSION

This paper has presented a unique derivation for a nonparabolic hydrodynamic transport model. This approach utilized moment operators to reveal simplifying assumptions and to arrive at more compact mathematical formu-

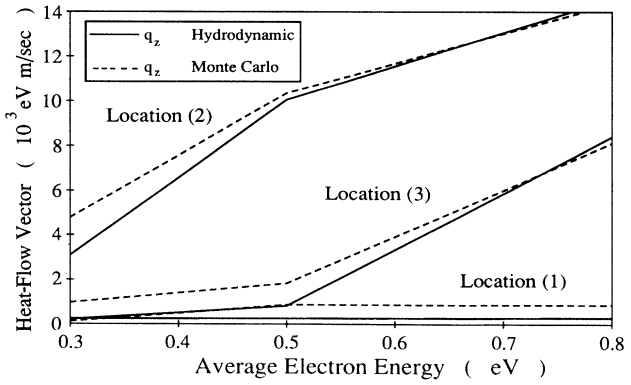

FIG. 10. Γ-valley heat-flow vector along the direction of applied electric field, at three locations within the ballistic diode, plotted as a function of applied bias. The other components were found to be negligibly small.

lation. This formulation was then used to postulate an improved ansatz distribution to close the moment equations and result in a model and nonparabolic transport of electrons in realistic semiconductor conduction bands. When combined with appropriate dissipation terms, this simplified model offers a computationally efficient method to model electron conduction in semiconductors. This type of model, which sacrifices some physical detail, leads to a more manageable mathematical problem with the potential of rapid solution generation using numerical methods.

Additionally, this paper presents an extensive Monte Carlo–based investigation into the applicability of this new model. The model parameters were tested in both stationary and nonstationary environments. In both cases the results are excellent. Hence this model should prove useful in investigating electronic-device structures. The model offers a method to better approximate electron transport with the potential of faster simulation times as compared to the more computationally intensive Monte Carlo technique.

ACKNOWLEDGMENTS

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